Toon Verstraelen

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Bond Dissociation & Electronegativity Equalization

It is well known that the *Electrongativity Equalization Mtehod* (EEM) fails to describe the charge distribution upon bond dissocation. In this presentation, the bond dissocation is studied with the *Atom-Condensed Kohn-Sham DFT approximated to second order* (ACKS2). After reviewing the basic equations, a two-fragment system is studied in the dissociation limit. The limiting behavior of the Coulomb interaction (1/r) and the Kohn-Sham matrix elements (exponentially decaying) are plugged into the equations. The solution exhibits integer dissocuation limits, in line with high-level ab initio computations. A direct fit of the ACKS2 model to reproduce constrained CAS-SCF reference data yield parameters that are in line with experimental atomic data.

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